2-Propanone, 1-phenoxy-

Other names:	Phenoxyacetone
	Phenoxymethyl methyl ketone
	1-Phenoxy-2-propanone
	1-Phenoxyacetone
	Phenoxy-2-propanone
Inchi:	InChI=1S/C9H10O2/c1-8(10)7-11-9-5-3-2-4-6-9/h2-6H,7H2,1H3
InchiKey:	QWAVNXZAQASOML-UHFFFAOYSA-N
Formula:	C9H10O2
SMILES:	CC(=O)COc1ccccc1
Mol. weight [g/mol]:	150.17
CAS:	621-87-4

Physical Properties

Property code	Value	Unit	Source
gf	-96.61	kJ/mol	Joback Method
hf	-237.36	kJ/mol	Joback Method
hfus	15.89	kJ/mol	Joback Method
hvap	47.06	kJ/mol	Joback Method
log10ws	-1.71		Crippen Method
logp	1.654		Crippen Method
mcvol	121.350	ml/mol	McGowan Method
pc	3439.94	kPa	Joback Method
ripol	1956.00		NIST Webbook
tb	502.70	K	NIST Webbook
tc	724.46	K	Joback Method
tf	289.77	K	Joback Method
vc	0.456	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.39	J/mol×K	508.29	Joback Method
cpg	269.00	J/mol×K	544.32	Joback Method
cpg	280.90	J/mol×K	580.35	Joback Method

cpg	292.11	J/mol×K	616.37	Joback Method
cpg	302.63	J/mol×K	652.40	Joback Method
cpg	312.50	J/mol×K	688.43	Joback Method
cpg	321.72	J/mol×K	724.46	Joback Method
dvisc	0.0023343	Pa×s	289.77	Joback Method
dvisc	0.0012799	Pa×s	326.19	Joback Method
dvisc	0.0007918	Pa×s	362.61	Joback Method
dvisc	0.0005347	Pa×s	399.03	Joback Method
dvisc	0.0003856	Pa×s	435.45	Joback Method
dvisc	0.0002925	Pa×s	471.87	Joback Method
dvisc	0.0002308	Pa×s	508.29	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C621874&Units=SI

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume